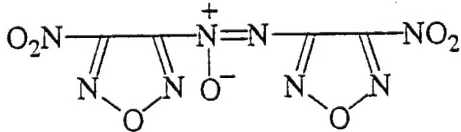


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Dr. Richard S. Miller

Technical Report No. 85

PREDICTED HEATS OF FORMATION OF DNAF  
IN GASEOUS, LIQUID AND SOLID PHASES

by

Peter Politzer, Jane S. Murray and M. Edward Grice

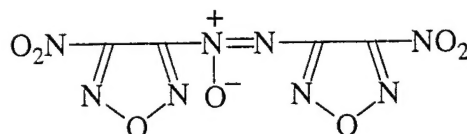
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October 10, 1995

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One of the compounds for which we have recently computed the gas phase heats of formation,  $\Delta H_f(\text{gaseous})$ , is DNAF, **1** [1]. This was done using our density functional procedure [2].



DNAF, **1**

In response to interest expressed by the Air Force Armament Laboratory (Eglin AFB), we have now estimated the liquid and solid phase heats of formation of **1**. For this purpose, we needed the heats of vaporization,  $\Delta H_{\text{vap}}$ , and sublimation,  $\Delta H_{\text{sub}}$ , which we obtained using general correlations between these properties and computed quantities related to electrostatic potentials on molecular surfaces [3].

$$\Delta H_f(\text{liquid}) = \Delta H_f(\text{gaseous}) - \Delta H_{\text{vap}} \quad (1)$$

$$\Delta H_f(\text{solid}) = \Delta H_f(\text{gaseous}) - \Delta H_{\text{sub}} \quad (2)$$

We found  $\Delta H_{\text{vap}} = 14$  kcal/mole and  $\Delta H_{\text{sub}} = 32$  kcal/mole. Then,

$$\Delta H_f(\text{gaseous}) = 169 \text{ kcal/mole} = 621 \text{ cal/g}$$

$$\Delta H_f(\text{liquid}) = 155 \text{ kcal/mole} = 570 \text{ cal/g}$$

$$\Delta H_f(\text{solid}) = 137 \text{ kcal/mole} = 504 \text{ cal/g}$$

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1. P. Politzer and M. E. Grice, Technical Report No. 78, Office of Naval Research, Contract No. N00014-95-1-0028, March 16, 1995.
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3. M. DeSalvo, E. Miller, J. S. Murray and P. Politzer, unpublished work.